

Structure-preserving nonlinear model reduction for finite-volume models

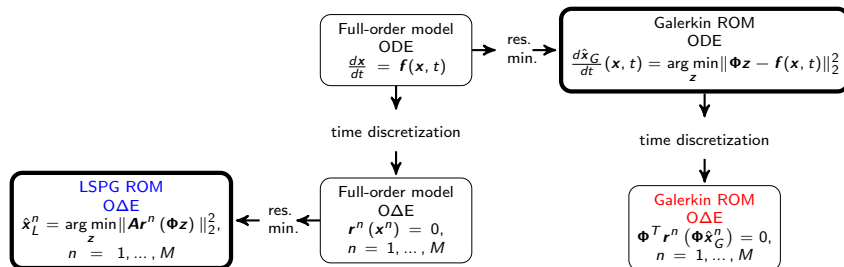
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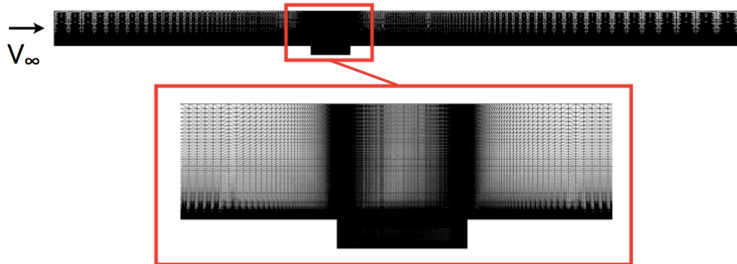
Optimize then discretize, or discretize then optimize?



- **Galerkin**: continuous-residual minimization
- **LSPG** [C. et al., 2011]: discrete-residual minimization

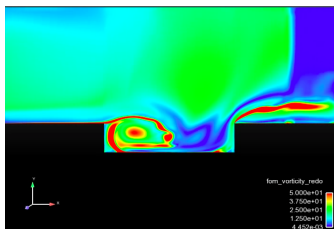
Comparative analysis: K. Carlberg, M. Barone, H. Antil, “Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction,” *Journal of Computational Physics*, 330:693–734, 2017.

Cavity-flow problem Collaborator: M. Barone (SNL)

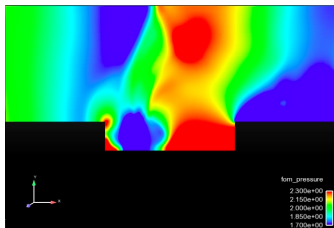


- Unsteady, compressible Navier–Stokes
- DES turbulence model
- Finite-volume discretization
- BDF2 linear multistep time integrator
- $M_\infty = 0.6$
- $\text{Re} = 6.3 \times 10^6$
- 1.2×10^6 degrees of freedom
- CFD code: AERO-F [Farhat et al., 2003]

Full-order model responses



vorticity field

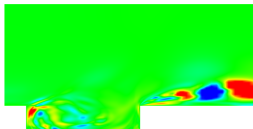


pressure field

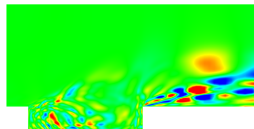
POD modes Φ (energy component)



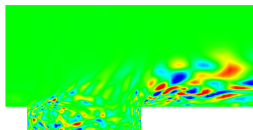
(a) mode 1



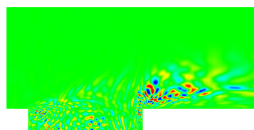
(b) mode 21



(c) mode 101

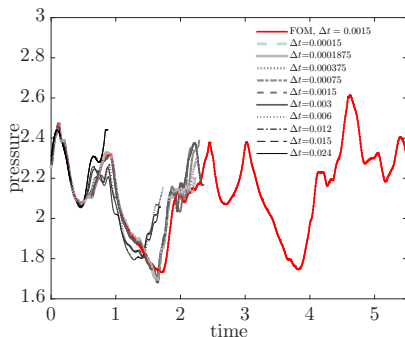


(d) mode 201

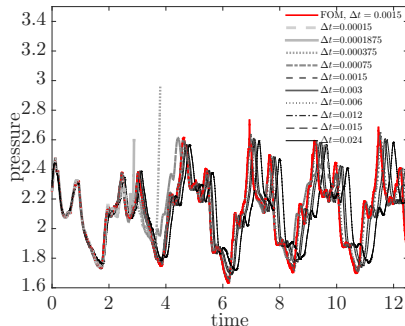


(e) mode 401

Galerkin and LSPG responses for basis dimension $p = 564$



(f) Galerkin



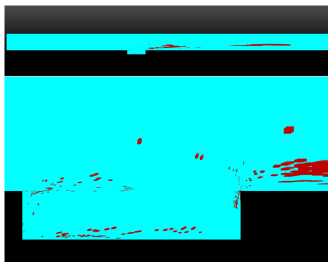
(g) LSPG

- Galerkin ROMs produce non-physical solutions
- LSPG ROMs
 - + accurate and stable (most time steps)
 - more expensive than the FOM (1.3 hours > 1 hour, 48 CPU)

Sample mesh [C. et al., 2013]

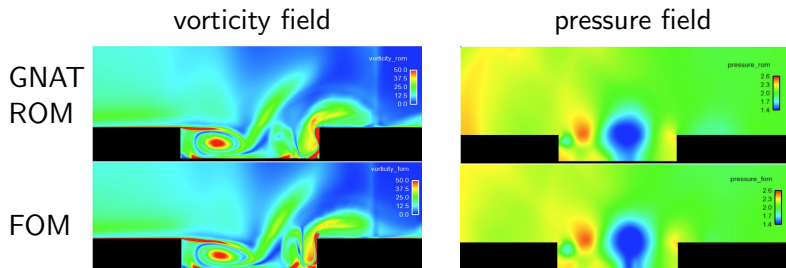
$$\hat{\mathbf{x}}^n = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \underbrace{\| (\mathbf{P}\Phi_R)^+ \mathbf{P} \mathbf{r}^n (\Phi \hat{\mathbf{z}}) \|_2^2}_{\mathbf{A}_{\text{GNAT}}}$$

- \mathbf{A}_{GNAT} : gappy POD [Everson and Sirovich, 1995] approx of residual
- *Sample mesh*: Extract mesh subset needed to compute $\mathbf{P} \mathbf{r}^n$
 - *Related*: RID [Ryckelynck, 2005], subgrid [Haasdonk et al., 2008]



- Sample mesh: 4.1% nodes, 3.0% cells
- + Small problem size: can run on many fewer cores

GNAT performance ($t \leq 12.5$ sec)



+ $< 1\%$ error in time-averaged drag

+ 229x CPU-hour savings

- FOM: 5 hour x 48 CPU
- GNAT ROM: 32 min x 2 CPU

Why is LSPG more accurate than Galerkin? [C. et al., 2017]

Theorem (Local *a posteriori* bounds: BDF schemes)

If the following conditions hold:

- 1 $\exists \kappa > 0$ such that $\|\mathbf{f}(\mathbf{x}, \cdot) - \mathbf{f}(\mathbf{y}, \cdot)\|_2 \leq \kappa \|\mathbf{x} - \mathbf{y}\|_2$,
 $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^N$
- 2 Δt small enough such that $0 < h := |\alpha_0| - |\beta_0| \kappa \Delta t$
- 3 A BDF scheme is employed for time integration, then

$$\|\delta \mathbf{x}_G^n\|_2 \leq \frac{1}{h} \|\mathbf{r}_G^n(\Phi \hat{\mathbf{x}}_G^n)\|_2 + \frac{1}{h} \sum_{\ell=1}^k |\alpha_\ell| \|\delta \mathbf{x}_G^{n-\ell}\|_2$$

$$\|\delta \mathbf{x}_L^n\|_2 \leq \frac{1}{h} \min_{\mathbf{y} \in \text{Ran}(\Phi)} \|\mathbf{r}_P^n(\mathbf{y})\|_2 + \frac{1}{h} \sum_{\ell=1}^k |\alpha_\ell| \|\delta \mathbf{x}_L^{n-\ell}\|_2$$

$$\blacksquare \delta \mathbf{x}_G^n := \mathbf{x}_\star^n - \Phi \hat{\mathbf{x}}_G^n.$$

$$\blacksquare \delta \mathbf{x}_L^n := \mathbf{x}_\star^n - \Phi \hat{\mathbf{x}}_L^n$$

LSPG minimizes the error bound sequentially in time!

Structure preservation in model reduction

- **Stability** [Moore, 1981, Bond and Daniel, 2008, Amsallem and Farhat, 2012, Kalashnikova et al., 2014]
- **Second order** [Freund, 2005, Salimbahrami, 2005, Chahlaoui, 2015]
- **Delay**
[Beattie and Gugercin, 2008, Michiels et al., 2011, Schulze and Unger, 2015]
- **Bilinear** [Zhang and Lam, 2002, Benner and Damm, 2011, Benner and Breiten, 2012, Flagg and Gugercin, 2015]
- **Inf-sup stability** [Rozza and Veroy, 2007, Gerner and Veroy, 2012, Rozza et al., 2013, Ballarin et al., 2014]
- **Passivity** [Phillips et al., 2003, Sorensen, 2005, Wolf et al., 2010]
- **Energy conservation**
[An et al., 2008, Farhat et al., 2014, Farhat et al., 2015]
- **Lagrangian structure** [Lall et al., 2003, C. et al., 2015]
- **(Port-)Hamiltonian** [Polyuga and van der Schaft, 2008, Beattie and Gugercin, 2011, Afkham and Hesthaven, 2016, Chaturantabut et al., 2016, Peng and Mohseni, 2016]

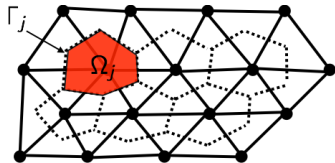
What structure should we preserve in finite-volume models?

Finite-volume discretization: full-order model

Full-order model ODE: $\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t)$

$$x_{\mathcal{I}(i,j)} = \frac{1}{|\Omega_j|} \int_{\Omega_j} u_i(\vec{x}, t) d\vec{x}$$

$$f_{\mathcal{I}(i,j)} = -\frac{1}{|\Omega_j|} \int_{\Gamma_j} u_i(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x}$$



- Conserved variables u_i , $i = 1, \dots, n_u$
- ℓ -component of velocity v_ℓ , $\ell = 1, \dots, d$ with $d \in \{1, 2, 3\}$
- ℓ -component of normal n_ℓ , $\ell = 1, \dots, d$
- $\mathcal{I} : \{1, \dots, n_u\} \times \{1, \dots, N_\Omega\} \rightarrow \{1, \dots, N\}$, $N = n_u N_\Omega$

Full-order model ODE: $\mathbf{r}^n(\mathbf{x}^n) = 0$, $n = 1, \dots, M$

$$r_{\mathcal{I}(i,j)}^n = \frac{1}{|\Omega_j|} \int_{\Omega_j} u_i(\vec{x}, t^{n+1}) - u_i(\vec{x}, t^n) d\vec{x} + \frac{1}{|\Omega_j|} \int_{t^n}^{t^{n+1}} \int_{\Gamma_j} u_i(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt$$

$r_{\mathcal{I}(i,j)}^n$: violation of conservation in u_i over Ω_j and $[t^n, t^{n+1}]$.

Finite-volume discretization: LSPG ROM

LSPG ROM: minimize $\| \mathbf{A} \mathbf{r}^n(\Phi \mathbf{z}) \|_2^2$

- + Minimizes (weighted) sum of squares of conservation-law violations
- Does not ensure conservation anywhere!



LSPG-FV ROM: minimize $\| \mathbf{A} \mathbf{r}^n(\Phi \mathbf{z}) \|_2^2$
 subject to $\bar{\mathbf{r}}^n(\Phi \mathbf{z}) = \mathbf{0}$

$$\bar{r}_{\bar{\mathcal{I}}(i,j)}^n = \frac{1}{|\bar{\Omega}_j|} \int_{\bar{\Omega}_j} u_i(\vec{x}, \mathbf{t}^{n+1}) - u_i(\vec{x}, \mathbf{t}^n) d\vec{x} + \frac{1}{|\bar{\Omega}_j|} \int_{\mathbf{t}^n}^{\mathbf{t}^{n+1}} \int_{\bar{\Gamma}_j} u_i(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt$$

- $\bar{\mathcal{I}} : \{1, \dots, n_u\} \times \{1, \dots, N_{\bar{\Omega}}\} \rightarrow \{1, \dots, \bar{N}\}$, with $\bar{N} = n_u N_{\bar{\Omega}}$
- + Minimizes sum of squares of conservation-law violations
- + Ensure conservation laws are enforced over $N_{\bar{\Omega}}$ subdomains

LSPG-FV: three cases

$$\blacksquare \mathbf{r}^n : \mathbb{R}^N \rightarrow \mathbb{R}^N$$

$$\blacksquare \boldsymbol{\Phi} \in \mathbb{R}_{\star}^{N \times p}$$

$$\blacksquare \bar{\mathbf{r}}^n : \mathbb{R}^p \rightarrow \mathbb{R}^{\bar{N}}$$

1 Underdetermined constraint problem ($p > \bar{N}$)

$$\underset{\mathbf{z}}{\text{minimize}} \|\mathbf{A}\mathbf{r}^n(\boldsymbol{\Phi}\mathbf{z})\|_2^2$$

$$\text{subject to } \bar{\mathbf{r}}^n(\boldsymbol{\Phi}\mathbf{z}) = \mathbf{0}$$

■ Solve with sequential quadratic programming (SQP)

+ Conservation over $\bar{\Omega}_j, j = 1, \dots, N_{\bar{\Omega}}$ ensured

2 Well-posed constraint problem ($p = \bar{N}$)

$$\bar{\mathbf{r}}^n(\boldsymbol{\Phi}\mathbf{z}) = \mathbf{0}$$

3 Overdetermined constraint problem ($p < \bar{N}$)

$$\underset{\mathbf{z}}{\text{minimize}} \|\mathbf{A}\mathbf{r}^n(\boldsymbol{\Phi}\mathbf{z})\|_2^2 + \mu \|\bar{\mathbf{A}}\bar{\mathbf{r}}^n(\boldsymbol{\Phi}\mathbf{z})\|_2^2$$

■ Penalty parameter $\mu \in \mathbb{R}_+$

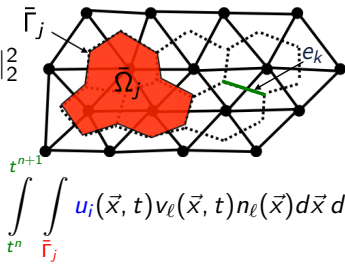
- No conservation guaranteed

Hyper-reduction

GNAT-FV ROM: $\min_{\mathbf{z}} \underbrace{\|(\mathbf{P}\Phi_R)^+ \mathbf{P}\mathbf{r}^n(\Phi\mathbf{z})\|_2^2}_{\mathbf{A}_{\text{GNAT}}}$
 subject to $\bar{\mathbf{r}}^n(\Phi\mathbf{z}) = \mathbf{0}$

$$\bar{r}_{\mathcal{I}(i,j)}^n = \frac{1}{|\bar{\Omega}_j|} \int_{\bar{\Omega}_j} u_i(\vec{x}, t^{n+1}) - u_i(\vec{x}, t^n) d\vec{x} + \underbrace{\frac{1}{|\bar{\Omega}_j|} \int_{t^n}^{t^{n+1}} \int_{\bar{\Gamma}_j} u_i(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt}_{\text{nonlinear flux}}$$

$$= \underbrace{\mathbf{a}(i,j)^T \Phi}_{\text{linear (precompute)}} (\hat{\mathbf{x}}^{n+1} - \hat{\mathbf{x}}^n) + \underbrace{\frac{1}{|\bar{\Omega}_j|} \int_{t^n}^{t^{n+1}} \mathbf{b}(i,j)^T \mathbf{g}(\mathbf{x}(t)) dt}_{\text{nonlinear}}$$



- Interface flux $\mathbf{g}_{\mathcal{J}(i,k)} = \int_{e_k} u_i(\vec{x}, t) v_\ell(\vec{x}, t) \bar{n}_\ell(\vec{x}) d\vec{x}$
- $\mathcal{J} : \{1, \dots, n_u\} \times \{1, \dots, N_e\} \rightarrow \{1, \dots, N_g\}$, with $N_g = n_u N_e$
- $\mathbf{a} : \{1, \dots, n_u\} \times \{1, \dots, N_{\bar{\Omega}}\} \rightarrow \mathbb{R}_+^N$
- $\mathbf{b} : \{1, \dots, n_u\} \times \{1, \dots, N_{\bar{\Omega}}\} \rightarrow \{-1, 0, 1\}^{N_g}$
- ℓ -component of edge normal \bar{n}_ℓ , $\ell = 1, \dots, d$

Approximate interface flux $\mathbf{g} : \mathbb{R}^N \rightarrow \mathbb{R}^{N_g}$ using gappy POD.

Hyper-reduction via Gappy POD [Everson and Sirovich, 1995]

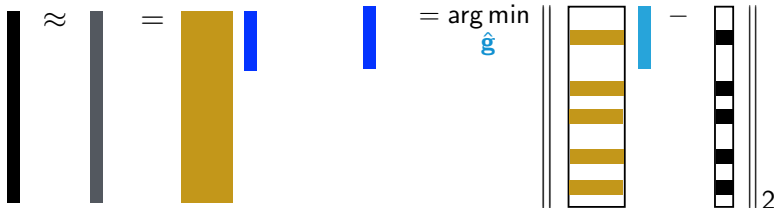
■ *Offline.* Compute:

1 $\Phi_g \in \mathbb{R}_*^{N_g \times n_g}$ (POD)

2 $P_g \in \{0, 1\}^{n_s \times N_g}$ (sample-mesh edges)

■ *Online.* Approximate flux via gappy POD:

1. $g(x) \approx \tilde{g}(x) = \Phi_g \hat{g}(x)$ 2. $\hat{g}(x) = \arg \min_{\hat{g}} \|P_g \Phi_g \hat{g} - P_g g(x)\|_2$

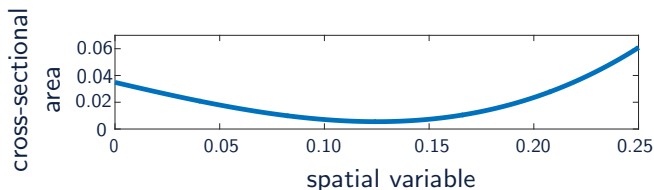


GNAT-FV ROM:
$$\min_z \|(\mathbf{P}\Phi_R)^+ \mathbf{P}r^n(\Phi z)\|_2^2$$

 subject to $\tilde{r}^n(\Phi z) = 0$

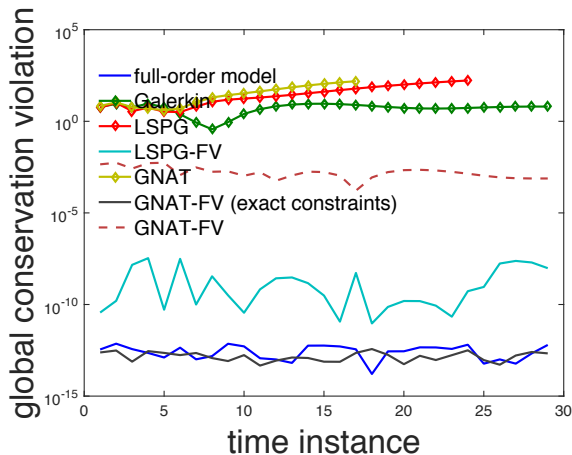
$$\tilde{r}_{\mathcal{I}(i,j)}^n = \underbrace{a(i,j)^T \Phi}_{\text{linear (precompute)}} (\hat{x}^{n+1} - \hat{x}^n) + \frac{1}{|\bar{\Omega}_j|} \int_{t^n}^{t^{n+1}} \underbrace{b(i,j)^T \Phi_g (P_g \Phi_g)^+}_{\text{linear (precompute)}} \underbrace{P_g g(x)}_{\text{sample flux}} dt$$

Example: Quasi-1D Euler equation



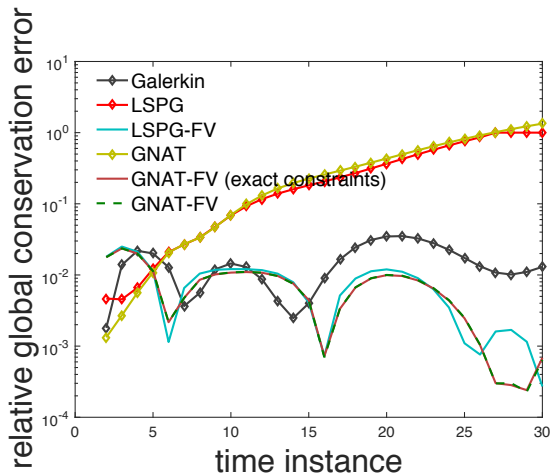
- $n_u = 3$ conserved quantities
 $\mathbf{u} = (\rho, \rho v, E)$
- Number of control volumes
 $N_\Omega = 100$
- Total time steps $M = 30$
- Time step $\Delta t = 0.01$
- Training: Mach number
 $M \in \{1.7, 1.8, 1.9, 2.0\}$
- Online: Mach number
 $M = 1.75$
- ROM parameters: $p = 5$,
 $n_g = 20$

Global conservation ($N_{\bar{\Omega}} = 1$)



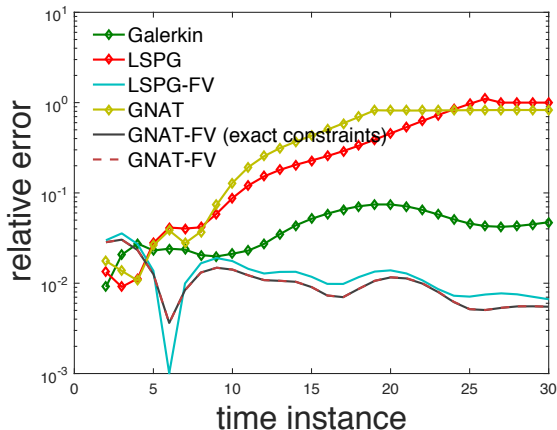
- + Global conservation exactly satisfied for exact constraints
- + GNAT-FV: accurate conservation-law approximation

Global conservation ($N_{\bar{\Omega}} = 1$)



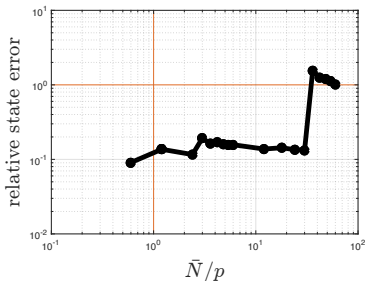
- Conservation-law constraints: **small** (but **nonzero**) error in globally conserved quantities

Global conservation ($N_{\bar{\Omega}} = 1$)

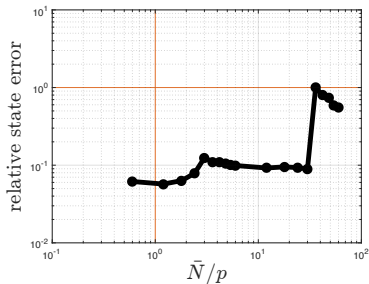


+ Relative state error roughly matches global conservation error

Varying number of subdomains $N_{\bar{\Omega}}$ (penalty parameter $\mu = 10^3$)



(h) LSPG-FV



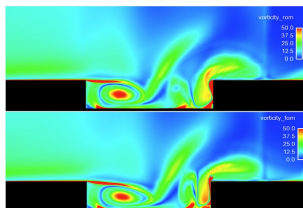
(i) GNAT-FV

- + Conservation-law constraints reduce error by $10\times$
- + GNAT-FV approximately the same accuracy as LSPG-FV
- + Best accuracy for global conservation ($N_{\bar{\Omega}} = 1$)

Conclusions

- Structure-preserving model reduction for nonlinear finite-volume models
 - Conservation-law violation equality constraints
 - Enforces conservation over subdomains
 - Hyper-reduction by applying gappy POD flux approximation
- Numerical experiments
 - + Constraints reduced both state and global conservation errors
 - Best results obtained for **global conservation** ($N_{\tilde{\Omega}} = 1$)

Questions?

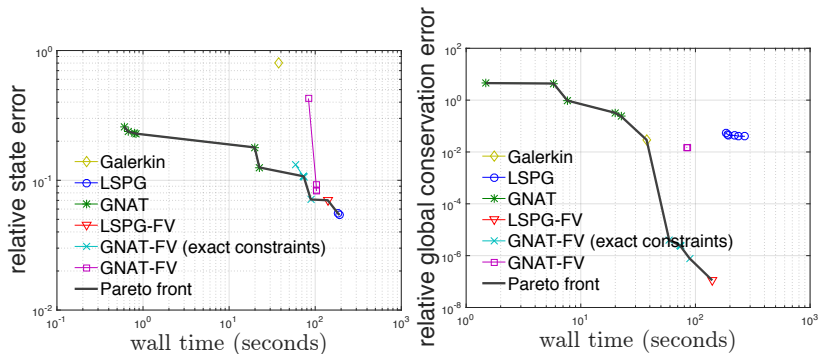


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Acknowledgments

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- GNAT: Pareto optimal for small wall times
- + GNAT-FV, LSPG-FV: Pareto optimal for smaller errors



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